Scalable High-Order Multi-Material ALE Simulations

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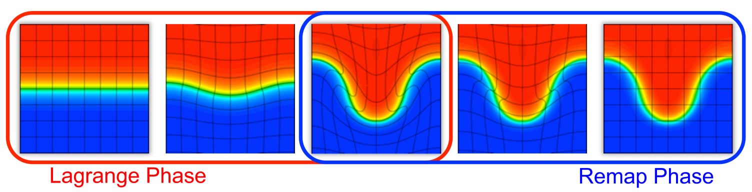
Abstract: BLAST is a mutli-material ALE hydrodynamics code which implements the high-order finite element formulations of [1,2,3,4] and is based on the finite element software library, MFEM [5]. We consider recent performance optimizations to the code which target both the sparse and dense linear algebra components of the high-order ALE algorithm and show good strong scaling properties. We also highlight recent developments and applications of the algorithm in challenging multi-material ALE simulations.

Text

The BLAST Multi-Material ALE Algorithm

BLAST solves the Euler equations using a high-order finite element ALE formulation based on three phases:

- **Lagrangian phase**: solve on moving curvilinear mesh
- **Mesh optimization phase**: harmonic or inverse-harmonic smoothing
- **Remap phase**: conservative and monotonic DG advection based remap



On a semi-discrete level our method can be written as

	Lagrangian Phase	Remap Phase
Material:	$\mathbf{M}\frac{d\boldsymbol{\eta}_k}{dt} = \mathbf{b}_k$	$\mathbf{M}\frac{d\boldsymbol{\eta}_k}{d\tau} = \mathbf{K}\boldsymbol{\eta}_k$
Mass:	$\eta_k\rho_k\lvert\mathbf{J}\rvert = \eta_k^0\rho_k^0\lvert\mathbf{J}^0\rvert$	$\mathbf{M}\frac{d(\boldsymbol{\eta\rho})_k}{d\tau} = \mathbf{K}(\boldsymbol{\eta\rho})_k$
Energy:	$\mathbf{M}_{\mathbf{e_k}}\frac{d\mathbf{e}_k}{dt} = \mathbf{F}_k^T \cdot \mathbf{v}$	$\mathbf{M}\frac{d(\boldsymbol{\eta\rho}\mathbf{e})_k}{d\tau} = \mathbf{K}(\boldsymbol{\eta\rho}\mathbf{e})_k$
Momentum:	$\mathbf{M_v}\frac{d\mathbf{v}}{dt} = -\mathbf{F}\cdot\mathbf{1}$	$\mathbf{M_v}\frac{d\mathbf{v}}{d\tau} = \mathbf{K_v}\mathbf{v}$

where $\mathbf{F}$ is the rectangular force matrix, $\boldsymbol{\eta}_k$, $\boldsymbol{\rho}_k$, $\mathbf{e}_k$ are the indicator, density and energy for material k with discontinuous basis ϕ and $\mathbf{v}$ is the velocity with continuous vector basis w.
The mass and advection matrices are defined as:

$$(\mathbf{M})_{ij} = \int_\Omega \phi_i\phi_j, \quad (\mathbf{M}_{\mathbf{e_k}})_{ij} = \int_\Omega \eta_k\rho_k\phi_i\phi_j, \quad (\mathbf{M_v})_{ij} = \int_\Omega \rho w_j w_i,$$

$$(\mathbf{K}_\rho)_{ij} = \sum_z \int_z u\cdot\nabla\phi_j\phi_i - \sum_f \int_f (u\cdot n)[\![\phi_j]\!](\phi_i)_d, \quad (\mathbf{K_v})_{ij} = \sum_z \int_z \rho u \cdot \nabla w_j w_i$$

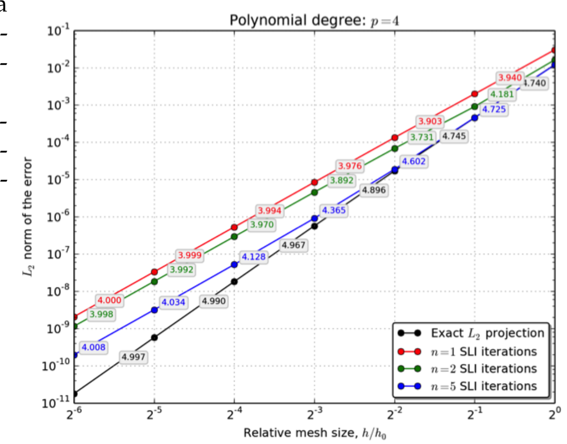
The algorithm has memory bandwith bound kernels involving distributed, sparse matrices and compute bound kernels involving local, dense matrices.

SLI improves Sparse Linear Solver Perfromance

The momentum equations in the Lagrange and Remap phases require solving a sparse, global linear system which is a **memory bandwidth bound kernel**.

PCG is typically used where a global (parallel) reduction is required after each iteration to compute residuals.
An alternative approach is Stationary Linear Iteration (SLI), a sequence of improving approximations based on mass lumping:

- $B_1 = M_L^{-1}$
- $B_2 = 2M_L^{-1} - M_L M M_L^{-1}$
- $\dots$
- $I - B_n M = (I - M_L^{-1}M)^n$

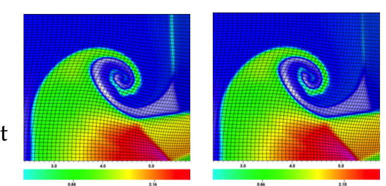


SLI has attractive properties:

- Convergence:

$$\lim_{n\to\infty} B_n = M^{-1}$$

- Mass conservative
- Small, fixed iteration count
- No global reduction

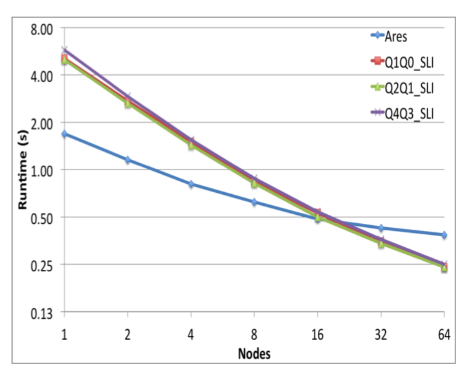


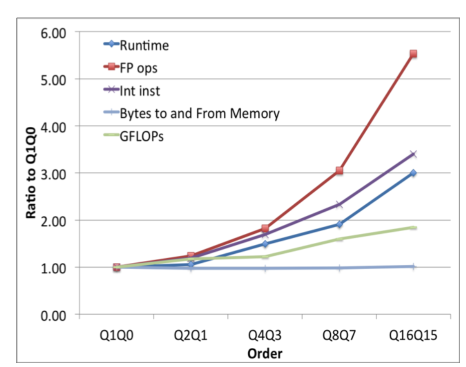
Analytic projection using SLI (top), Q2 ALE using PCG (left) versus 4 iterations of SLI (right)

Optimizations for Dense Linear Algebra Kernels

The force matrix $\mathbf{F}$ is assembled from zonal matrices $\mathbf{F}_z$. Calculating each $\mathbf{F}_z$ is a **compute bound kernel**. We have explored optimizations based on:

- Fixing small, dense matrix sizes at compile time (via templating) for substantial optimization imrpovements
- Use of "partial assembly" alogorithms which minimize data motion and integer instruction complexity as order is increased, at the expense of more floating point

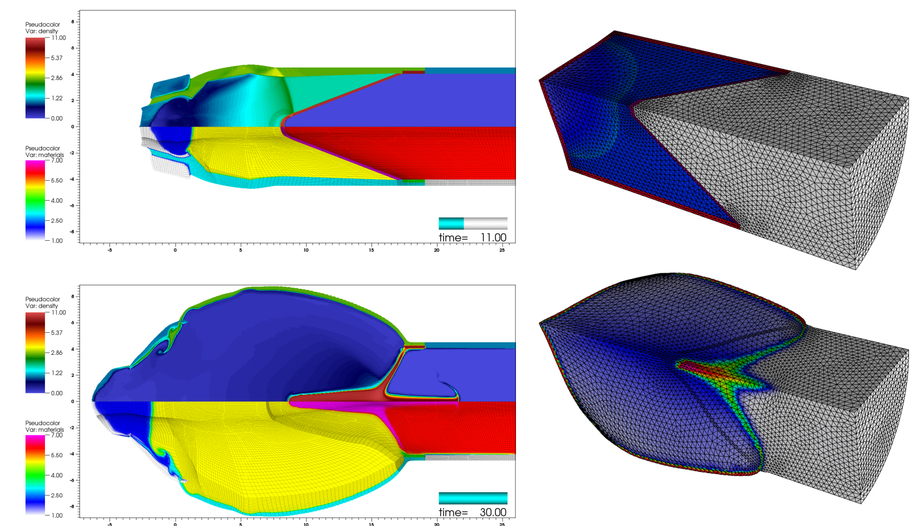




Strong parallel scaling comparrison to ARES code for 2D sedov benchmark (left) and growth of FP, memory, runtime as a function of order for fixed DoF count (right)

Application to 2Drz/3D Multi-material ALE Simulations

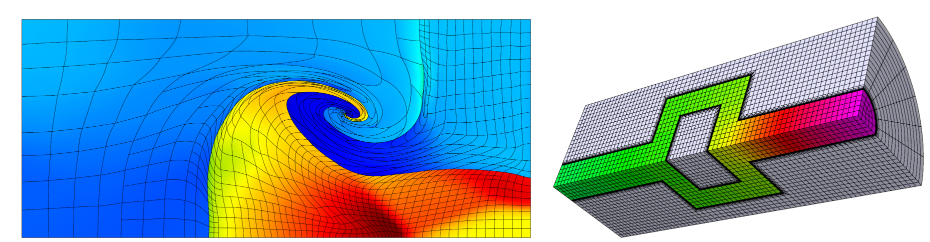
BLAST supports high-order multi-material ALE hydrodynamics on a wide variety of meshes, including curved tetrahedral elements.



BRL81 shaped charge simulation in 2Drz using Q2 ALE (left) and simplified shaped charge in 3D using Q2 ALE on a curved tetrahderal mesh (right).

Current Research and Development Efforts

We continue to research and develop new methods and capabilities:



Example of preliminary static, non-confroming mesh refinement capability (left) and Q2 H(Div) single group radiation diffusion on the crooked pipe benchmark (right)

References

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[3] V. Dobrev, Tz. Kolev, and R. Rieben, High order curvilinear finite elements for elastic-plastic Lagrangian dynamics, *Journal of Computational Physics*, **257B**, pp. 1062-1080, 2014

[4] R. Anderson, V. Dobrev, Tz. Kolev and R. Rieben, Monotonicity in High-Order Curvilinear Finite Element ALE Remap, *Int. J. Numerical Methods in Fluids*, **77(5)**, pp. 249-273, 2015

[5] MFEM library, `http://mfem.org`